Polar bosons in one-dimensional disordered optical lattices

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We analyze the effects of disorder and quasi-disorder on the ground-state properties of ultra-cold polar bosons in optical lattices. We show that the interplay between disorder and inter-site interactions leads to rich phase diagrams. A uniform disorder leads to a Haldane-insulator phase with finite parity order, whereas the density-wave phase becomes a Bose-glass at very weak disorder. For quasi-disorder, the Haldane insulator connects with a gapped generalized incommesurate density wave without an intermediate critical region.

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Introduction. The interplay between disorder and interactions plays a crucial role in the physics of strongly-correlated systems [1]. Disorder in non-interacting systems leads to Anderson localization [2], which in one dimension occurs for vanishingly small disorder [3]. For the particular case of bosons in a lattice potential, interactions have been shown, both in 1D [4–7] and higher dimensions [8, 9], to induce in the presence of disorder a phase diagram characterized by three phases: a superfluid (SF) phase, a gapless localized incompressible phase known as Bose-Glass (BG), and a Mott-insulator (MI) occuring at commesurate lattice fillings.

Ultra-cold atoms in optical lattices offer an extraordinarily controllable scenario for the detailed analysis of the competition between disorder and interactions. Disorder in the on-site energies may be implemented in various ways in these systems, including the use of speckle [10–13], binary mixtures [14–17], and bichromatic combinations of two mutually incommensurate lattices [18]. Recently, localization has been experimentally observed in non-interacting cold gases in 1D and 3D speckle [19–21], and bichromatic potentials [22]. Bichromatic lattices constitute a peculiar type of disorder, rather a quasi-disorder, realizing the so-called Aubry-André model [23]. The effects of interactions in 1D lattices with quasi-disorder have been recently studied [24–27]. Particularly interesting is the existence of a gapped localized phase, the so-called incommensurate density wave (ICDW), which results from the quasi-periodicity of the potential.

Polar gases are attracting a growing attention mostly motivated by experiments on atoms with large magnetic moments [28–30], and especially by recent groundbreaking experiments on polar molecules [31]. Due to the dipole-dipole interaction, these gases present an exceedingly rich physics [32, 33]. Polar lattice gases are particularly interesting, mostly due to the qualitatively new features introduced by dipole-induced inter-site interactions [34]. In particular, inter-site interactions may allow for the realization of the so-called Haldane-insulator (HI) phase [35], a gapped phase characterized by a nonlocal string order parameter.

In this Letter we show that the interplay between on-site and inter-site interactions and disorder leads to a rich physics for lattice bosons with nearest neighbor interactions. In particular, in the presence of uniform disorder the HI phase is preserved, although with finite parity, up to a finite disorder, where a phase transition into a BG is produced. On the contrary, in the presence of quasi-disorder the HI is connected, without any intermediate critical region, to a gapped generalized ICDW phase occurring for non-polar gases. Other phases are discussed in detail for both types of disorder.

Model. As mentioned above, the main qualitatively new feature of polar lattice gases concerns the significant inter-site interactions. Polar interactions between sites placed $j > 0$ sites apart decay as $1/j^3$. Although interactions for $j > 1$ do play a role in the physics of polar gases, especially in what concerns the existence of crystalline phases at any fractional filling (Devil's staircase [36, 37]) for very weak on-site interactions and sufficiently large dipoles, the most relevant properties of polar lattices gases may be understood from a model with only nearest-neighbor interactions:

$$\begin{aligned} H &= -t\sum_i (b_i^\dagger b_{i+1} + H.c.) + \frac{U}{2}\sum_{i=1}^{N} n_i(n_i-1) \\ &\quad +V\sum_i n_i n_{i+1} + \sum_i \epsilon_i n_i, \end{aligned} \tag{1}$$

with $b_i^\dagger$, b_i the creation/annihilation operators for bosons at site i, $n_i = b_i^\dagger b_i$, t the hopping amplitude, U (V) the on-site (inter-site) interaction, and ϵ_i the on-site energy.

In the following we consider an average filling factor $n = 1$. Assuming small deviations from this average, we may introduce an effective spin via the standard Holstein-Primakoff (HP) transformation $S_i^z = \delta n_i = 1 - n_i$, $S_i^+ = \sqrt{2-n_i}\,b_i$. The resulting spin Hamiltonian resembles to a large extent an antiferromagnetic spin-1 XXZ model with uniaxial single-ion anisotropy (the mapping is however imperfect, especially at low U, due to occupations $n > 2$, and extra terms appearing when introducing the HP transformation):

$$H = J\sum_i \left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z + D(S_i^z)^2 \right], \tag{2}$$

with $J = 2t$, $D = U/4t$, and $\Delta = V/2t$. For $D > 0$ and $\Delta > 0$ three ground-state phases are possible [38], a Néel

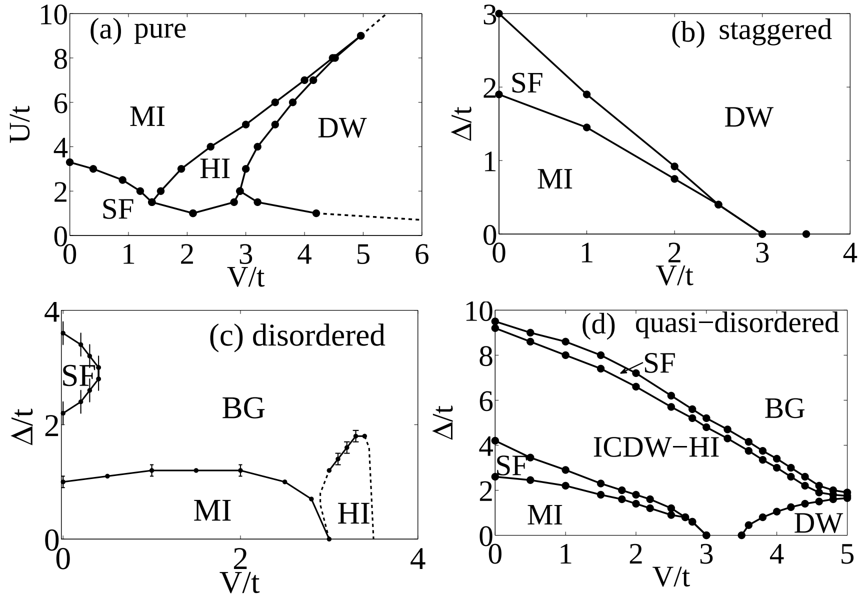

FIG. 1: Phase diagrams of bosons with nearest-neighbor interactions: (a) unperturbed case; (b) staggered on-site energy; (c) uniform disorder; (d) quasi-disorder. Figures (b)–(d) are obtained for $U/t = 5$. See text for details.

antiferromagnet (AF) for sufficiently large $\Delta > 0$, a large-D phase for dominant single-ion anisotropy, and the gapped Haldane phase [39] characterized by a non-local string-order [40].

Unraveling the HP transformation, the equivalent bosonic phases are: a density wave (DW) phase, characterized by a finite $\mathcal{O}_{DW} = \lim_{|i-j|\to\infty}\langle(-1)^{i-j}\delta n_i \delta n_j\rangle$, and a static structure factor $S(k) = \frac{1}{N^2}\sum_{i,j} e^{ik(i-j)}\langle n_i n_j\rangle$ (with N the number of sites) peaked at $k = \pi$; a MI with hidden parity order $\mathcal{O}_P = \lim_{|i-j|\to\infty}\langle(-1)^{\sum_{i<l<j}\delta n_l}\rangle$ [41] (recently measured in site-resolved experiments [42]); and a Haldane-insulator (HI) phase, with finite string-order $\mathcal{O}_S = \lim_{|i-j|\to\infty}\langle\delta n_i(-1)^{\sum_{i<l<j}\delta n_l}\delta n_j\rangle$ [35, 41]. Density-matrix renormalization group (DMRG [43]) calculations for soft-core polar bosons [35, 41] have shown that indeed a HI occurs in a window $V_c^{(1)}(U) < V < V_c^{(2)}(U)$ [44]. At large U a direct first-order MI-DW transition occurs. All the previous phases are insulating, being characterized by an exponentially decaying single-particle correlation function $G(r) = \langle b_i^\dagger b_{i+r}\rangle/\sqrt{\langle n_i\rangle\langle n_{i+r}\rangle}$ [25]. At low U occupations $n > 2$ break down the boson-spin mapping, and a superfluid (SF) phase may be found, which is a Luttinger-liquid characterized by an algebraically decaying $G(r) \propto r^{-1/2K}$. A MI to SF Kosterlitz-Thouless (KT) transition occurs at sufficiently low U and V when the Luttinger parameter $K > 2$ [41, 45]). The MI-HI Gaussian transition line is a Luttinger-liquid with Luttinger parameter $2 > K_c(U) > 1/2$ [41]. At low U but large V our DMRG calculations show a DW to SF transition with a critical $K = 1/2$ [45] (Fig.1a). Below the HI region we find as well a SF region for $K > 2$.

Numerical method. We employ below DMRG calculations with open boundary conditions for determining the ground-state phases for different types of disorder. Special care must be taken with the edge states in the HI phase, which are polarized by adding one more particle or eliminated by coupling two extra hard-core bosons at the chain edges in order to form a singlet state [46]. Both procedures destroy the energy gap for the MI and ICDW phases. We hence introduce two different definitions for the gap to the first excited state, E_G and E'_G, which are respectively calculated without and with the mentioned polarization/elimination procedure. For the MI and ICDW, $E_G \neq 0$ and $E'_G = 0$; for HI and DW by $E_G = 0$ and $E'_G \neq 0$; and for the gapless phases (SF and BG) $E_G = E'_G = 0$. The Luttinger exponent K of the SF phases is extracted by fitting the single-particle correlation function $G(r)$ using finite-size conformal corrections [47]. The number of particles is conserved and the maximal bosonic occupation per site is $n_{max} = 8$ for $U \neq 0$ [48]. We consider lattice sizes of $N = 55$, 89, 144 and 233 sites (see discussion below). The number of optimal states kept in the DMRG ranges from 300 to 500. Statistical deviations are particularly relevant in the case of uniform disorder discussed below. For that case we have performed up to 60 realizations per case (we refer to the supplementary material for a discussion on the error bars). We have checked that our results converge to the exact values in the non-interacting limit (where we keep $n_{max} = N$), and to earlier calculations for interacting systems with $V = 0$ [6] (see the supplementary material).

Staggered potential. As a starting point we first consider the case of a commesurate staggered on-site energy $\epsilon_i = (-1)^i\Delta$, which resembles the case of staggered magnetic fields in spin chains. For the latter case it is known [49, 50] that the Haldane phase is continuously connected to the AF phase. Due to the explicit symmetry breaking, the AF phase is a singlet and not a doublet, and a Gaussian transition occurs between large-D and AF phases. We hence expect that the HI phase continuously connect to the DW phase for even

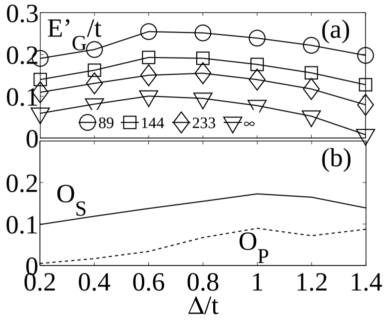

FIG. 2: (a) Gap E'_G as a function of Δ for the uniform disorder case with $U = 5t$, $V = 3.3t$, and different lattice sizes; (b) For the same parameters, string-order $\mathcal{O}_S$ and parity-order $\mathcal{O}_P$, for $N = 144$.

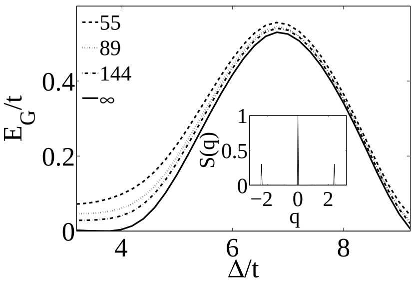

FIG. 3: Excitation gap of the ICDW as a function of Δ for the quasi-disordered case with $U = 5t$ and $V = 0$, and different lattice sizes; (inset) Static structure factor $S(q)$ for $\Delta = 7t$ ($N = 144$); $S(q)$ presents side-peaks corresponding to the $1/(1-\beta)$ quasi-periodicity.

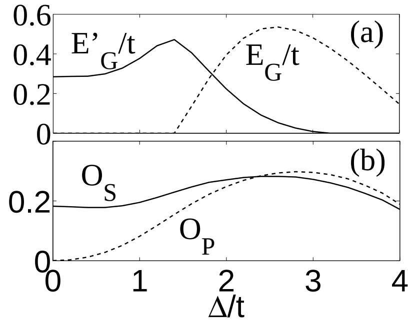

FIG. 4: (a) Gaps E_G and E'_G (extrapolated to infinite-size systems from our results for $N = 55$, 89 and 144) as a function of Δ for the quasi-disordered case with $U = 5t$, and $V = 3.3t$; (b) For the same parameters, string-order $\mathcal{O}_S$ and parity order $\mathcal{O}_P$, for $N = 144$

vanishingly small Δ, as observed in our numerical simulations (Fig. 1(b)). Note that a finite SF region opens for the bosonic case between the MI and the DW phases.

Uniform disorder. We consider next a uniform disorder, in which ϵ_i has a uniform random distribution in the interval $[-\Delta, \Delta]$. The presence of disorder induces a gapless localized Bose-Glass (BG) phase [4, 5, 8], separating the MI and the SF phase. At unit filling, and intermediate U values, for growing Δ a MI-BG transition is followed by a BG-SF transition, and a final SF-BG transition at larger Δ , the SF-BG boundary forming a characteristic finger-like shape [6, 7]. The SF-BG boundary is characterized by a Luttinger parameter $K = 3/2$ [4, 5]. Our numerics recover these well-known results for $V = 0$ (see Fig. 1(c) and the supplementary material). For growing V the intermediate SF region shrinks and eventually vanishes, whereas the MI phase stretches up to a critical $V = V_c^{(1)}$, which marks the MI-HI transition for $\Delta = 0$. Close to $V_c^{(1)}$ numerical calculations cannot resolve whether a BG opens at the MI-HI boundary for vanishingly small disorder. Although RG calculations to the lowest order predict a stable MI-HI boundary at weak disorder[51], RG calculations using $4k_F$ terms to the density [52, 53] show that a BG should appear at the MI-HI boundary at vanishingly small disorder for $K < 3/2$ and at finite disorder for $K > 3/2$. For the value $U/t = 5$ in the figure, $K = 1.18$ and we hence expect a BG region all the way to vanishing disorder.

For $V_c^{(1)} < V < V_c^{(2)}$ we obtain that a gapped phase survives up to a critical Δ given approximately by the Haldane-like gap at $\Delta = 0$ (Figs. 1(c) and 2(a)). This phase presents a finite $\mathcal{O}_S$. The survival of this gapped phase for finite uniform disorder resembles the persistence of the Haldane phase for weak random magnetic fields in spin-1 chains [51, 52, 54]. This phase however is characterized by a finite $\mathcal{O}_P$ which grows with increasing Δ (Fig. 2(b)). Whereas in the pure HI phase $\mathcal{O}_P = 0$ due to the fluid-like spatial distribution of defects $\delta n = \pm 1$, the finite $\mathcal{O}_P$ relates to the growing localization of defects with increasing disorder, while still keeping string order. Resorting to the language of "solid-on-solid" models [40], we may map defects $\delta n = \pm 1$ into spin-$1/2$ particles, and sites with $\delta n = 0$ as empty sites. In this analogy the pure HI phase would be an AF-spin-ordered fluid, whereas the DW phase would be an AF-spin-ordered solid. The Haldane-like phase in the presence of disorder could be understood as an AF-spin-ordered glass-like in this analogy.

On the contrary the DW is destroyed even for very weak disorder, similar to the destruction of the AF phase in spin-1 chains [51, 52]. This results from the proliferation of domain walls in accordance with the Imry-Ma argument [55]. Our results show for $V > V_c^{(2)}$ a large reduction of the gap for $\Delta \ll V$, as well as the expected domain formation. However, the convergence of the gap towards zero with the system size is very slow, since the length of the Imry-Ma domains scales as $1/\sqrt{\Delta}$, and hence much larger lattice sizes are demanded to observe the gap destruction at very weak disorder.

Quasi-disorder. We consider at this point the case of quasi-disordered potentials. Such potentials may be easily generated in ultra-cold gases by means of bichromatic lattices [22, 56], in which a second lattice incommensurate with the first lattice is added. In that case the system experiences an on-site energy $\epsilon_j = \Delta \cos(2\pi\beta j + \phi)$, in which β characterizes the incommesurability of both lattices, and Δ is given by the potential depth of the second lattice. In the following we consider $\beta = (\sqrt{5} - 1)/2$. The chain length is chosen following the Fibonacci series $N = 55, 89, 144, 233$ in order that the potential is closest to be periodic with N. We have checked that in most cases the results are not affected by the choice of ϕ, and we hence set $\phi = 0$ in the following.

As mentioned above, it has been recently shown [24, 25] that quasi-periodic potentials allow for an ICDW, which is a localized but gapped phase, contrary to the BG. The ICDW may be understood from the beating of both lattice frequencies which leads to super-wells with a characteristic length scale $1/(1-\beta)$. A filling $1-\beta$ (or β) hence leads to the formation of an approximate density wave. For filling factor $n=1$, a possibly gapped localized phase (i.e. a generalized ICDW) may occur as well, and a MI-SF-ICDW-SF-BG scenario cannot be excluded [25]. Our results for $V=0$ show a clearly gapped localized ICDW whose gap converges to a finite value when extrapolating to infinite size (Fig. 3). This phase is characterized by a peak in the static structure factor $S(k)$ given by the approximate $1/(1-\beta)$ periodicity (inset of Fig. 3). Hence, at $V=0$ we observe a MI-SF-ICDW-SF-BG phase diagram (Fig. 1(d)). The last SF region is rather narrow, and within numerical accuracy it is compatible with a critical line. At the SF-MI transitions we obtain numerically $K \simeq 1$, compatible with results obtained for spinless fermions [57]. For the SF-ICDW transitions we find as well $K \simeq 1$. For $V < V_c^{(1)}$ the MI-SF-ICDW-SF-BG topology is maintained, but the MI and low SF regions shrink vanishing at $V_c^{(1)}$.

For $V_c^{(1)} < V < V_c^{(2)}$ and low Δ, we obtain as for the uniform disorder case a HI phase with growing $\mathcal{O}_P$ when Δ increases (Fig. 4 [58]). This is again due to the growing localization of defects $\delta n = \pm 1$ by the quasi-disorder while keeping string-order. However, contrary to the uniform disorder case, the quasi-disordered case allows for the generalized ICDW phase which has also finite $\mathcal{O}_S$ and $\mathcal{O}_P$. As a consequence, the increasing pinning of defects for increasing Δ leads to a connection between HI ($E'_G > 0$) and generalized ICDW ($E_G > 0$), without any gapless region in between (Fig. 4). Our DMRG calculations, including the determination of fidelity susceptibility [59], show that the generalized ICDW and the HI phases form an overall gapped region. Finally, for $V > V_c^{(2)}$ we observe the opening of a finite DW region, which contrary to the uniform disorder case is not immediately destroyed at small Δ. The DW region undergoes at finite Δ an Ising transition into the generalized ICDW phase.

Conclusions. In summary, uniform disorder and quasi-disorder lead to rather different phase diagrams for polar bosons in optical lattices. For uniform disorder a HI phase with finite parity survives up to a finite disorder where a HI-BG transition occurs, whereas the DW phase becomes a BG for any finite disorder. On the contrary, in the presence of quasi-disorder the HI phase continuously connects with a generalized ICDW phase without any intermediate critical region, and the DW survives up to a finite disorder. The predicted phases may be detected using state of the art techniques. In particular, the string order may be detected using similar site-resolved techniques as those recently employed for the detection of non-local parity order in MI phases [42].

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Supplementary material for "Polar bosons in one-dimensional disordered optical lattices"

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In this supplementary material we briefly comment on the determination of the error bars for the case of uniform box disorder.

We determine the SF-BG boundary by monitoring the behavior of the single-particle correlation function $G(r)$, which has a power-law decay in the SF phase. This decay can be fitted very well using conformal field corrections for open boundary conditions, allowing for the calculation of the corresponding Luttinger parameter K. The SF-BG phase boundary is determined at the point in which $K = 3/2$ [1]. In order to benchmark our calculations we have established the phase diagram for disorded non-polar gases. Figure 1 shows that the calculated SF-BG boundary is in excellent quantitative agreement with that obtained in Ref. [2] using quantum Monte Carlo techniques.

In order to determine the error bars, we have studied for different V and Δ up to 60 disorder realizations. We randomly pick different sub-sets of these realizations and average for each sub-set the correlation $G(r)$. The error bars indicate for a given V the regime of Δ values in which for some, but not all, sub-sets correlations are best fitted by a power-law with $K = 3/2$.

We establish the error bars between gapped and gapless phases, i.e. MI-BG and HI-BG using a similar procedure. We evaluate again a large number of disorder realizations for different lattice sizes. We perform finite-size scaling to obtain the excitation gap. The error-bar region is that at which some disorder realizations present finite gap whereas other realizations are not gapped.

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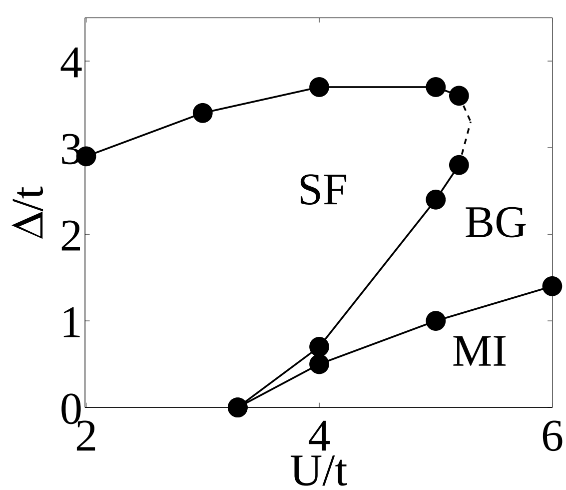

FIG. 1: Phase diagram for the non-polar Bose-Hubbard model with uniform box disorder, for a chain length $L = 89$, with 30 disorder realization per point.